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K-Levels in Axially Deformed Nuclei with Relativistic Hartree-Bogoliubov Theory

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Abstract. Relativistic density functionals provide a powerful phenomenological way to study nuclear structure phenomena. They have been mostly used in describing bulk nuclear properties of ground states and have been also very successful in the description of collective excitations. Nuclear excitations that form due to the inherent structure of nuclei and have a relatively long half-life are called isomers. They play a significant role in recent experimental and theoretical studies of nuclei far from stability, in nuclear fission and in the process of nucleosynthesis relative to astrophysics. In this study we concentrate on the single particle excitations of high K-level isomers that appear mainly at nuclei with well defined axial deformation. We employ the blocking effect to create two quasiparticle states within the relativistic hartree-Bogoliubov framework. We use the Equal filling approximation that respects the time-reversal symmetry breaking caused by blocking. We concentrate our interest in medium mass axially deformed nuclei where there have been several experimentally observed K-level isomers and we can compare directly our results.

1 Introduction

The term isomers in nuclear physics is used to describe excited states with relatively long lifetimes compared to either the ground states or other excited states in the same area. Usually, nuclear excited states have a lifetime of the order of 10^{-12} sec, however isomer lifetimes can be 100 to 1000 times longer, with some extreme cases of seconds, to minutes or even years [1, 2]. Isomers also have a crucial role in recent experimental and theoretical studies of nuclei far from stability [3, 4], which are presently at the forefront of nuclear science.

The decay of isomers can happen in very different ways, as nuclear excited state, i.e. γ-emission, β-decay, electron conversion, α-decay or fission. The transition

probability of each decay path can be affected by several factors such as the excitation energy and the symmetry of the excited configuration. More specifically, the intrinsic structure of isomeric states leads to an increased lifetime. As the nuclear matrix elements of the transition operator, for the otherwise straightforward decay path, are connected with large changes of particular quantum numbers the corresponding decay would be hindered. In well deformed heavy nuclei the angular momentum quantum number K along the symmetry axis plays an important role. Levels with high K-values (*K-level isomers*) can only decay through γ-transitions of very high multipolarity with very small transition probability.

The theoretical approach mostly used for the study of K-levels, is the macroscopic-microscopic configuration constrained model [5–8]. Relativistic density functional theory has also been used in the transactinide region in [9].
In the present work we use the relativistic functionals DD-ME2 [10] and DD-PC1 [11] within the Hartree-Bogoliubov framework for the creation of two-quasipartilce states that represent the K-level excitations of the ground state. Of special interest are even-even nuclei with well deformed axial shape and in the region of Hf-, Er- isotopes ($A \approx 180$) [12, 13], where there has been great experimental effort to study their existence [14].

2 Isomer Formation

K-levels are a special case of low lying isomers of single particle nature. They are mainly observed in well deformed heavy nuclei, where the projection of the total angular momentum K on the symmetry axis is a good quantum number. They can form for large values of quadrupole deformation, where orbitals with high values of total angular momentum j come close to the Fermi surface. Therefore, with a small amount of energy approximately equal to the energy required for the breaking of a nucleon pair, it is possible to create excited states of two quasiparticles, involving configurations combining such high-j orbitals. In Table 1 we show the most common configurations of this kind that appear in specific regions.

In order to study K-levels we use the blocking effect within the Hartree-Bogoliubov framework creating two-quasiparticle states. Starting from the ground state $|\Phi_0\rangle$ of a nucleus which is defined as the quasiparticle vacuum i.e.

$$\alpha_k|\Phi_0\rangle = 0 \quad \text{for} \quad E_k > 0 \quad \text{or} \quad |\Phi_0\rangle = \prod_{E_k>0} \alpha_k|-\rangle, \tag{1}$$

where $|-\rangle$ is the bare vacuum of the configuration space defined by the original single particles, we create two-quasiparticle states that in principle correspond to low lying excitations of the initial system,

$$|\Phi_2\rangle = \alpha_1^\dagger \alpha_2^\dagger |\Phi_0\rangle \tag{2}$$

Table 1. Common two quasiparticle configurations in prolate deformed nuclei, in medium to heavy and superheavy regions.

Neutrons	Protons
$Z \sim 70 - 74$ $N \sim 100 - 108$	
$6^- : 5/2^-[512], 7/2^+[633]$	
$6^+ : 5/2^-[512], 7/2^-[514]$	
$6^+ : 5/2^+[642], 7/2^+[642]$	$6^+ : 5/2^+[402], 7/2^+[404]$
$8^- : 9/2^+[624], 7/2^-[514]$	$8^- : 9/2^-[514], 7/2^+[404]$
$Z \sim 102 - 108$ $N \sim 150 - 164$	
$8^- : 7/2^+[624], 9/2^-[734]$	$8^- : 7/2^-[514], 9/2^+[624]$
$8^- : 7/2^+[613], 9/2^-[734]$	
$10^- : 9/2^+[615], 11/2^-[725]$	$10^- : 9/2^-[505], 11/2^+[615]$

The new state represents the vacuum of the set of quasiparticle operators

$$(\alpha'_1, \alpha'_2, \ldots, \alpha'_N) \tag{3}$$

where N is the dimension of the quasiparticle space with

$$\alpha'_1 = \alpha^\dagger_1,\ \alpha'_2 = \alpha^\dagger_2,\ \ldots, \alpha'_N = \alpha_N. \tag{4}$$

In this way a new quasiparticle basis is formed defined by the set of operators $(\alpha'_1, \ldots, \alpha'_N, \alpha'^\dagger_1, \ldots, \alpha'^\dagger_N)$, with the exchange of operators $\alpha^\dagger_1 \leftrightarrow \alpha_1$, $\alpha^\dagger_2 \leftrightarrow \alpha_2$. In other words, the application of the blocking effect is equivalent with the exchange of the annihilation operators $\alpha_1,\ \alpha_2$ with the creation operators $\alpha^\dagger_1,\ \alpha^\dagger_2$ corresponding to the quasiparticle states with the lowest energies, or in the single particle picture to the states that are closer to the Fermi surface.

Typically the study of even-even nuclei with the solution of the RHB equations is simplified by time-reversal symmetry, with the time reversed states being degenerate. In axially deformed nuclei this means that orbitals with opposite signs of angular momentum projection Ω will have the same energy. This fact significantly reduces the computational effort needed for the solution of the RHB equations, by cutting in half the dimension of the matrix representation of the equations. However, the procedure that creates the two quasiparticle states lifts this specific degeneracy. Formally, the blocking of a state means that at the same time the state with the opposite sign of Ω should be forced to be unoccupied. In this case one should use the full dimension of the RHB equations. In order to avoid this complication we will be using the equal filling approximation [15–17] which allows us to apply the blocking effect without breaking the time reversal symmetry

Practically, this means that in each step, the density matrix ρ is averaged and the pairing tensor κ is symmetrized for the K sub-spaces where blocking takes

place and are replaced by the equations

$$\rho' = \rho + \frac{1}{2}(U_{k_b} U^{*T}_{k_b} - V^{*}_{k_b} V^{T}_{k_b}), \quad (5)$$

$$\kappa' = \kappa - \frac{1}{2}(U_{k_b} V^{*T}_{k_b} + V^{*}_{k_b} U^{T}_{k_b}), \quad (6)$$

where U_{k_b} and V_{k_b} correspond to the Bogoliubov coefficients U and V of the blocked quasiparticle level.

3 Results

Based on the theoretical framework we developed, we follow a specific sequence to obtain the energy of the isomer we want to study. We start from the solution of the RHB equations for the ground state of a certain nucleus. We then identify the position of the two orbitals that form the configuration that has the required quantum numbers and solve the RHB equations, this time by blocking these specific states. The excitation energy of the isomer is the difference of the total energy calculated between the ground state and the two quasiparticle state.

The single particle spectrum around the Fermi surface is crucial in order to understand the evolution of the energies of single particle excitations, in a chain of isotopes. Some key features are the absolute energy value of each state and the position of the two states that create the isomer relative to the Fermi surface, since the sum of their respective quasiparticle energies is a first approximation of the isomeric energy. In general, in the neutron spectrum the Fermi surface moves upward as we go to the next isotope. This means that the quasiparticle energy of each neutron state changes between different isotopes. On the other hand the relative position of the Fermi surface stays constant in the proton spectrum. Naturally, as the number of neutrons increases, the whole spectrum is shifted downwards due to the extra binding of the additional neutrons.

In order to compare with the experimentally observed energies of a specific *K*-level isomer, we calculate the energy difference from all the possible low lying configurations and in the end keep the one that gives the lowest energy.

3.1 6^+ isomer in Hf isotopes and $N = 104$ isotones

3.1.1 Hf isotopes

In this section we will show the results from the study of the formation of 6^+ *K*-level isomer, which is systematically observed in Hf isotopes and in $N = 104$ isotones. We start with the isotopic chain of $^{170-180}$Hf. The two quasiparticle configurations that can create a 6^+ isomer based on Table 1 are: $\nu 5/2^-[512] \otimes \nu 7/2^-[514]$ and $\nu 5/2^+[642] \otimes \nu 7/2^+[633]$ for neutrons and $\pi 5/2^+[402] \otimes \pi 7/2^+[404]$ for protons. In references [12, 14], for the four isotopes $^{170-176}$Hf

the 6^+ isomer is formed by the two neutron states $\nu 5/2^-[512] \otimes \nu 7/2^-[514]$ while in the ^{178,180}Hf is formed by the two proton states $\pi 5/2^+[402] \otimes \pi 7/2^+[404]$. Within our model the only difference is that the lowest energy for the 6^+ isomer in ^{170,174}Hf comes from the neutron configuration $\nu 5/2^+[642] \otimes \nu 7/2^+[633]$.

In Table 2 we show the numerical results of the calculation of the 6^+ isomer, in the first column for the DD-ME2 force, in the second the DD-PC1 and in the last column we give the experimental values [12]. Figure 1 is a schematic representation of these results.

Table 2. 6^+ isomer energy in Z = 72 Hf isotopes

	DD-ME2	DD-PC1	Expt.
170 Hf	2.217	2.528	1.773
172 Hf	2.116	2.487	1.685
174 Hf	1.891	1.931	1.549
176 Hf	1.437	1.574	1.333
178 Hf	2.569	2.905	1.554
180 Hf	3.096	3.120	1.703

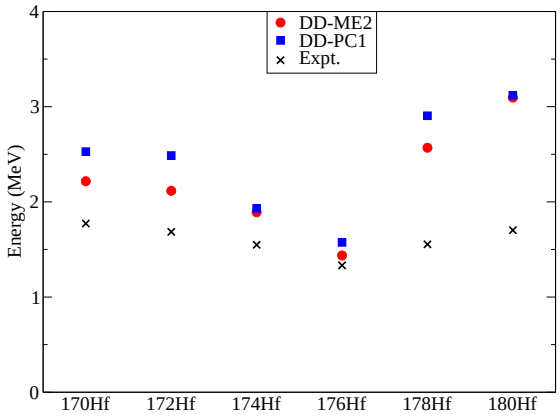

Figure 1. Evolution of the 6^+ isomer in Hf isotopes, for the functionals DD-ME2 and DD-PC1, compared with the experimental data.

In general we observe that the evolution of the theoretical prediction of the energy shows the same structure as the experimental values. It gradually decreases until its lowest value which experimentally is at 1.333 MeV in ^{176}Hf and then it increases again. Quantitatively, the two functionals have similar results, with the DD-PC1 giving slightly larger values for the first four isotopes and slightly lower for the last two. The first four isotopes where the calculated values come from the blocking of two neutron states, reproduce more accurately the experimental value, while in the last two isotopes the difference between theory and

experiment is around 1 MeV. There is also an abrupt increase in these two energies. This is to be expected based on the details of the single particle spectra, particularly from the distance of the Fermi surface or equivalently at the relative energy difference of the states blocked to form the isomer. Specifically, for the ^{178,180}Hf isotopes, the absolute energy difference of the two proton states $\pi 5/2^+[402]$ $\pi 7/2^+[404]$, is close to 2.7 MeV and the position of the particle state $\pi 5/2^+[402]$ is relatively high with two and three states lying between this state and the Fermi level. For the ^{170,172}Hf isotopes, the corresponding energy difference between the states $\nu 5/2^+[642]$ $\nu 7/2^+[633]$ is smaller and around 2 MeV and for the ^{174,176}Hf isotopes the $\nu 5/2^-[512]$ and $\nu 7/2^-[514]$ states are even more close with only 1 MeV separating them. Additionally, for these four lighter isotopes the respective states sit more closely to the Fermi surface with only one other state interceding.

This shows that an important property for the correct numerical prediction of the excitation energy, is the initial position in the ground state of the two levels that create the isomer and the energy difference between them. In other words, it is important that these states are the ones with the lowest quasiparticle energies in the ground state.

3.1.2 $N = 104$ isotones

The same procedure is applied for the study of the 6^+ isomer in $N = 104$ isotones with $68 \leq Z \leq 76$, which in all nuclei comes from the combination of $\nu 5/2^-[512] \otimes \nu 7/2^-[514]$.

Since now the neutron number is fixed, the relative position of these two states with the Fermi level does not change significantly from one isotone to the other. More specifically, in the calculated single particle spectrum one sees that the neutron orbit $5/2^-[512]$ is located at the same place directly above the Fermi energy, as the total spectrum is shifted downwards with increasing Z. In addition, the $7/2^-[514]$ neutron state is the first hole state below the Fermi energy for the first two nuclei ^{172}Er and ^{174}Yb while for the other three nuclei it is second with $7/2^+[633]$ in between. Furthermore, the energy difference and hence the sum of their quasiparticle energies increases gradually from 0.4 Mev to 1.2 MeV, something we expect to appear in the calculation of the isomeric energy.

Indeed, in Table 3 where we compare the theoretical and the experimental values in the same way as in Table 2, one sees the gradual increase of the 6^+ isomer energy, with the exception of the experimental value of ^{176}Hf where there is a downward kink. This becomes more obvious in Figure 2 which is a schematic representation of our results. The increase of the experimental energies is less pronounced with $\sim$ 0.3 MeV more from the first to the last nucleus, where for the two functionals this increase is $\sim$ 0.5 MeV. Also, in all isotones the experimental value is always relatively higher, with the DD-ME2 results being

Table 3. 6^+ isomer energy from n5/2- n7/2- 2qp configurations in $N = 104$ isotones

	DD-ME2	DD-PC1	Expt.
172 Er	1.135	1.174	1.500
174 Yb	1.251	1.266	1.518
176 Hf	1.534	1.296	1.333
178 W	1.539	1.576	1.665
180 Os	1.904	2.011	1.878

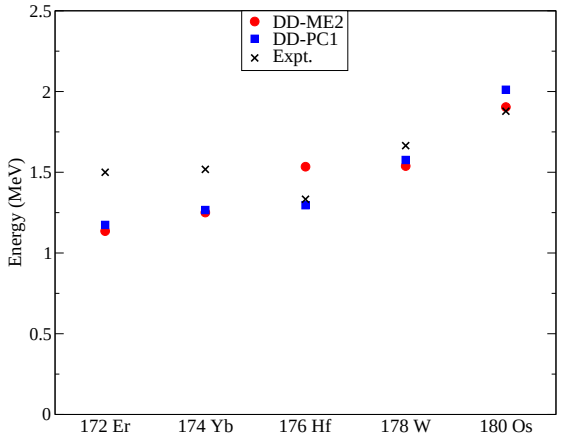

Figure 2. Evolution of the 6^+ isomer energy for the $N = 104$ as in Figure 1

closer than those coming from DD-PC1. Again ^{176}Hf is an exception since the theoretical values are much closer with experiment and DD-PC1 is closer than DD-ME2.

3.2 8^- isomer in Hf isotopes and in N=106 isotones

We now turn our interest to another systematically observed isomer. The 8^- level at Hf isotopes and the $N = 106$ isotones.

3.2.1 Hf isotopes

In the Hf isotopes the 8^- isomer comes from the two quasiproton configuration $\pi 9/2^-[514] \otimes \pi 7/2^+[404]$. From the calculated proton spectra of the isotopes we can deduce how these two states move along the isotopic chain. The $\pi 9/2^-[514]$ state starts as the second particle state above the Fermi surface in the first three nuclei ^{170,172,174}Hf. In ^{176}Hf it crosses the $\pi 1/2^-[541]$ state and for the rest of the nuclei it remains the closest particle state with its energy get-

ting closer to the Fermi level. The $\pi 7/2^+[404]$ starts as the third hole state below the Fermi level in ^{170}Hf where the states $\pi 1/2^+[411]$ and $\pi 1/2^-[541]$ are above it. For the ^{172}Hf it is the second hole state with only the $\pi 1/2^-[541]$ above. For all the other isotopes it is the closest hole state and its distance from the Fermi surface is also decreasing. As a whole, the energies of all the states move downwards with increasing N, while the gap between the states $\pi 9/2^-[514]$ and $\pi 7/2^+[404]$ is gradually getting smaller from ~ 2.5 MeV to ~ 0.5 MeV, as they both come closer to the Fermi surface.

Applying the blocking procedure for these two states we can examine how the energy of the 8^- level, changes along the Hafnium isotopic chain. In Table 4 we show for each isotope the values of the excitation energy as it is calculated with DD-ME2 and DD-PC1 and the experimental value given in Ref. [14]. The corresponding diagram is given in Figure 3.

The structure of the single particle spectrum is imprinted in the calculated energy

Table 4. 8^- isomer energy from p7/2+ p9/2- 2qp configurations in Hf isotopes

	DD-ME2	DD-PC1	Expt.
170Hf	2.865	3.226	2.183
172Hf	2.618	3.027	2.005
174Hf	2.160	2.607	1.798
176Hf	1.816	2.228	1.559
178Hf	1.532	1.812	1.350
180Hf	1.335	1.697	1.142
182Hf	1.191	1.534	1.173
184Hf	1.086	1.434	1.272
186Hf	1.334	1.797	-

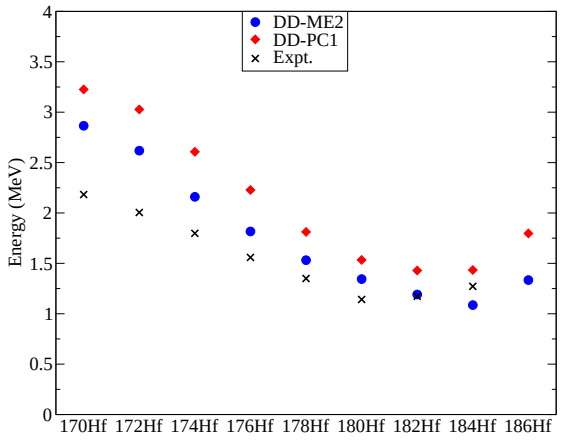

Figure 3. Evolution of the 8^- isomer energy in the Hf isotopes

and in Figure 3 and it explains the pattern of the experimentally observed energy. More specifically, the experimental values start at 2.183 MeV for ^{170}Hf they decrease linearly losing about 0.2 MeV at each subsequent isotope, until ^{180}Hf which has the minimum value and then increase for the last two nuclei where the 8^- has been experimentally measured. A similar pattern is observed for the theoretical values, they start at around $\approx$ 2.5 MeV and gradually lose energy coming closer to the experiment, the difference is that the lowest energy appears in ^{184}Hf and not in ^{180}Hf. The result for the ^{186}Hf has been included so that one can see that indeed in ^{184}Hf is the theoretical minimum. This behavior is common for the two functionals that show similar results.

3.2.2 N=106 isotones

The last case of a systematically observed isomer is the 8^- level in the even-even $N = 106$ isotones with $68 \leq Z \leq 82$. Although, not all of the nuclei in this series are well axially deformed, since ^{184}Pt is a transitional nuclei while ^{186}Hg shows oblate-prolate shape coexistence and ^{188}Pb is a neutron-deficient nuclei, still an excited level with quantum numbers 8^- has been experimentally observed in all of them [12] coming from the $\nu 7/2^-[514] \otimes \nu 9/2^+[624]$ configuration.

In the calculated single particle energy spectrum of the corresponding nuclei in their ground states, we observe the following details. In general as we move to heavier nuclei all the orbitals move to lower energies. Especially for the neutrons spectra as we increase the number of protons the position of the Fermi level with respect to other levels is the same. For the $\nu 9/2^+[624]$ state, its relative position to the rest of spectrum is stable, being the first of the particle states for all the isotones examined and its energy getting slightly closer to the Fermi level. On the other hand the $\nu 7/2^-[514]$ state moves away from the Fermi level and it also changes its relative position. For ^{174}Er as well as ^{176}Yb it is the second hole state, with the orbit $\nu 5/2^-[512]$ being right above. For the rest of the nuclei it is shifted to a lower relative position going deeper in the spectrum, always located below the $\nu 7/2^+[633]$ orbit. In total the energy difference or the equivalent sum of quasiparticle energies between those two states is increasing from one isotone to the next. The results of the calculation of the energy of a two quasiparticle state coming from the blocking of these states are shown in Table 5 and schematically in Figure 4.

Concentrating on the experimental observation of the 8^- level excitation energy, we see that it follows an irregular pattern with an increasing energy from 1.112 MeV to 2.578 MeV. What is very interesting is that the theoretical calculations which are practically equivalent for both functionals, reproduce this irregular pattern. However, quantitatively they give values that are larger by about 0.8–1 MeV. Hence, the calculated excitation energy is $\approx$ 1.9 MeV at ^{174}Er and is increased to $\approx$ 3.6 MeV at ^{188}Pb. This picture is explained by examining

Table 5. 8^- isomer energy from $\nu 7/2^-[514] \otimes \nu 9/2^+[624]$ 2qp configurations in N = 106 isotones

	DD-ME2	DD-PC1	Expt.
174 Er	2.174	2.232	1.112
176 Yb	2.037	2.003	1.050
178 Hf	2.418	2.373	1.147
180 W	2.694	2.645	1.529
182 Os	2.894	2.887	1.831
184 Pt	3.052	2.971	1.839
186 Hg	3.595	3.665	2.217
188 Pb	3.525	3.675	2.578

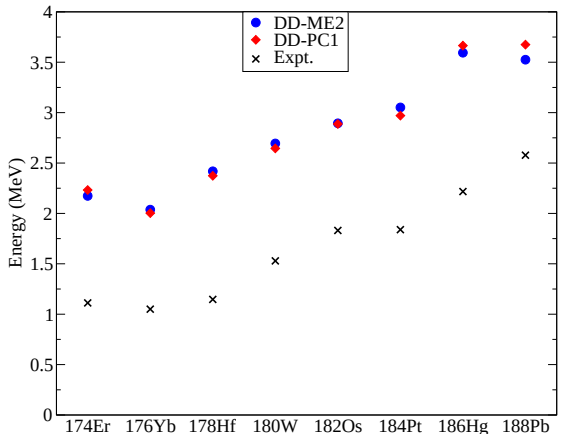

Figure 4. Evolution of the 8^- isomer energy in the $N = 106$ isotones

the details of the quasiparticle energies of the ground states. In particular one sees that, the quasiparticle energy corresponding to $\nu 9/2^+[624]$ is the lowest for each isotone with the exception of ^{174}Er and its value shows a small reduction up to ^{184}Pt. In addition, the quasiparticle energy of $\nu 7/2^+[633]$ is the fourth lowest and shows an increase again up to ^{188}Pb, with a variation that resembles the irregular pattern of the experiment.

4 Conclusions

The focus of this study has been the phenomenon of the creation of *K*-level isomeric excited states, in heavy nuclei with axially deformed shape of prolate type. *K*-level isomers are metastable excited states, that owe their relatively large half-life to the conservation of the large value of K, i.e. the projection of the total angular momentum on the symmetry axis. For the theoretical investigation the

generalised framework of the relativistic Hartree-Bogoliubov approach, has been extended to include the blocking effect for the creation of two quasiparticle states within the equal filling approximation. In this way, it has been made possible to compare theoretical calculations of the *K*-level isomer energies from self-consistent mean-field theories with corresponding known and well established experimental data in medium weight nuclei with $A \approx 160 - 190$ and in the region of Er to Pb ($68 \leq Z \leq 84$, $98 \leq N \leq 112$).

The main conclusion from the evaluation of this particular theoretical approach, is that it provides the ability to interpret the qualitative characteristics of the systematic appearance of specific isomers in the nuclear chains that have been examined. More specifically, the corresponding underlying single-particle structure calculated within our model, allowed for the explanation of the observed variation that the experimental values of the examined isomers show, through the different series of nuclei. In this context very important are, the relative position of the two orbits that create the isomer with the Fermi surface, as well as the change of the energy difference between them or equivalently the sum of their respective quasiparticle energies.

As it was shown, a better quantitative description of the experimental results exists in the cases of nuclei, where the two quasiparticle states that form the isomer, are the closest to the Fermi energy. In the rest of the nuclei where in the corresponding spectrum there are states with lower quasiparticle energy there is an important difference between the theoretical prediction and the experimental value. This might be a consequence of a general prediction of relatively large energy gaps between the neutron or proton shells, as they occur from relativistic mean-field models. This fact indicates the necessity of the inclusion of additional correlations possibly beyond the mean-field for a more accurate description of the phenomenon. For example, it is important to note that the approximation we followed, conserves the time reversal symmetry which is in principle broken by the blocking procedure. Effectively, the unpaired nucleons that create the isomer state, interact with the average nuclear field. This interaction has not been included at the calculation of the energies as presented above. One approach is to approximate this interaction as a small perturbation of the mean field and simulate its effect. This could be part of a future research plan, for a better description of *K*-level isomers within covariant density functionals.

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